JOURNAL OF COMPLEXITY 17, 898–909 (2001)
doi:10.1006/jcom.2001.0617, available online at http://www.idealibrary.com on IDEAL®

Numerical Integration of Harmonic Functions with Restricted Sampling Data

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Received January 26, 2001; revised May 23, 2001; accepted June 8, 2001

Based on the idea of kriging and the radial basis function approximation, we develop in this paper a numerical scheme to integrate harmonic functions with restricted sampling data. To be more precise, the integration is performed by using the function values which are given as discrete sampling data on only part of the boundary. These problems often arise from non-destructive evaluation techniques in the engineering industry. The existence and uniqueness of the solution and the error estimation for the proposed numerical scheme are also discussed. Several numerical experimental results are presented for the verification on the accuracy and convergence of the method. © 2001 Elsevier Science

Key Words: kriging; radial basis; weighted linear approximation; inverse problem.

[1] Supported by the National Science Foundation of China (Project 19971017) and the Croucher Foundation of Hong Kong.

[2] The work described in this paper was partially supported by a grant from the Research Grants Council of the Hong Kong Special Administrative Region, China (Project 9040428).

0885-064X/01 $35.00

1. INTRODUCTION

Consider the problem on how to numerically integrate a $(d+1)$-variate function

$$u\colon [-1, 1]^d \times [0, 1] \to R$$

under a very restrictive condition that the function values are not given in the domain $[-1, 1]^d \times [0, 1]$, but rather given at some discrete points $\{(x_j, 0)\}_{j=1}^n$ on only part of the boundary $[-1/2, 1/2]^d \times [0, 0]$. These problems often arise from the non-destructive evaluation techniques in the engineering industry [1, 3, 8, 9]. Usually the function u satisfies some kinds of partial differential equations in the domain. Here, we assume that the function u satisfies the Laplace's equation and is therefore harmonic in the domain $[-1, 1]^d \times [0, 1]$. We also assume that the values of the function and its normal derivatives can only be sampled on part of the boundary. This problem can be formulated as the following Cauchy problem of partial differential equations,

$$\begin{aligned} \Delta u(x, y) &= 0, \qquad \text{for} \quad x \in [-1, 1]^d, \quad y > 0, \\ u(x, 0) &= f(x), \qquad x \in [-1, 1]^d, \\ \frac{\partial u(x, 0)}{\partial y} &= g(x), \qquad x \in [-1, 1]^d, \end{aligned} \tag{1}$$

where Δ is the Laplacian operator. In real applications, we can only measure the Cauchy data $\{f(x_j)\}_{j=1}^n$ and $\{g(x_k)\}_{k=n+1}^{n+m}$, where $x_j, x_k \in [-1/2, 1/2]^d$. The problem is to calculate the multiple integral

$$\int_{[0, 1]} \int_{[-1, 1]^d} u(x, y)\, dx\, dy. \tag{2}$$

Since $\Delta u(x, y) = 0$, we have

$$\frac{\partial^{\alpha+\beta} u}{\partial x^\alpha\, \partial y^\beta} = -\frac{\partial^{\alpha+\beta} u}{\partial x^{\alpha+2}\, \partial y^{\beta-2}}, \qquad \forall \alpha \geqslant 0, \beta \geqslant 2.$$

All the partial derivatives of $u(x, y)$ with respect to x and y on the boundary $[-1/2, 1/2]^d \times [0, 0]$ can then be represented by the derivatives of $f(x)$ and $g(x)$ with respect to x, providing that the function $u(x, y)$ is harmonic on the boundary too. In other words, any harmonic function $u(x, y)$ can be uniquely determined from the boundary condition (1) via

Taylor expansion and harmonic extension. Problem (1) is then a limiting case of the above argument. See Bukhgeim *et al.* [4] for details on the existence, uniqueness and stability of the problem (1). Due to the highly ill-posedness of the problem, most numerical methods fail to produce an acceptable numerical solution. The reason is due to the fact that the problem can be treated as the classical Cauchy problem for the Laplace's equation, which is extremely sensitive to the initial Cauchy data $f(x)$ and $g(x)$. Recently, Cheng *et al.* [5] and Hon *et al.* [6] proposed a new numerical method for solving the Cauchy problem Laplace's equation in a two-dimensional case through a transformation of the Cauchy problem to a moment problem whose numerical approximation can be achieved.

The approach we want to demonstrate in this paper comes from the concept of kriging, which is equivalent to the radial basis approximation given in [12]. For further discussion about kriging and the radial basis interpolation, see Matheron [7], Powell [10], and Wu and Schaback [12–14].

The radial basis function space consists of all functions of the form $\sum_{j=1}^{n} \lambda_j \phi(\|x-x_j\|)$, where ϕ: $R_+ \to R$ is a given univariate function. The use of the univariate function in principle saves the computational time for evaluating the approximation of the solution. This numerical advantage is particularly important in handling multivariate problems.

2. METHODOLOGY AND ALGORITHM

Poisson's kernel is defined by the kernel function

$$P(x, y) = C_d \frac{y}{(\|x\|^2 + y^2)^{\frac{d+1}{2}}}, \tag{3}$$

where C_d is a constant which depends on the dimension d and satisfies $\int_{R^d} P(x, y)\, dx = 1$. All bounded functions, which are harmonic on the upper half plane, can be represented by the following Poisson's integral (see [2]):

$$u(x, y) = \int_{R^d} u(t, 0)\, P(x-t, y)\, dt. \tag{4}$$

In the following we assume that the harmonic function u can always be represented by a Poisson's integral as given in (4). Based on the idea of

kriging [7, 12], we now assume that an approximation u^* to the solution u can be expressed as a linear combination of the given data as

$$u^*(x, y) = \sum_{j=1}^{n} a_j(x, y)\, f(x_j) + \sum_{k=n+1}^{n+m} b_k(x, y)\, g(x_k), \tag{5}$$

where $a_j(x, y)$ and $b_k(x, y)$ are functions to be determined. The multiple integral of the unknown solution $u(x, y)$ given in (2) can then be approximated by

$$\int_{[0,1]} \int_{[-1,1]^d} u^*(x, y)\, dx\, dy. \tag{6}$$

From Eq. (5), the multiple integral of $u^*(x, y)$ can be obtained by evaluating the multiple integrals of $a_j(x, y)$ and $b_k(x, y)$, which are independent of the unknown solution $u(x, y)$. We note here that this is different from the classical linear approximation method which seeks an approximation s from a function subspace S to the solution u such that $\|u-s\|$ is minimized under a certain norm. In order to overcome the ill-posedness of the problem, it is reasonable to require that the functions $a_j(x, y)$ and $b_k(x, y)$ are bounded and harmonic on the upper half plane. In other words, they can also be represented by the Poisson's integral as in (4). Since any function which is bounded and harmonic on the upper half plane can be uniquely determined by its value given on the boundary as shown in its Poisson's integral representation, the original Cauchy problem is equivalent (reduced) to finding an approximation $u^*(x, 0)$ of the form

$$u^*(x, 0) = \sum_{j=1}^{n} a_j(x, 0)\, f(x_j) + \sum_{k=n+1}^{n+m} b_k(x, 0)\, g(x_k) \tag{7}$$

to the solution $u(x, 0)$.

By expressing the functions $f(x)$ and $g(x)$ in the form of Poisson's integral and applying to the linear approximant (7), the problem turns out to be approximating $u(x, 0)$ by $u^*(x, 0)$, which can be represented as

$$u(x, 0) \simeq \lim_{s \to 0} \int_{R^d} \left(\sum_{j=1}^{n} a_j(x, 0)\, P(x_j - t, s) + \sum_{k=n+1}^{n+m} b_k(x, 0) \frac{\partial P(x_k - t, s)}{\partial s} \right) u(t, 0)\, dt. \tag{8}$$

This approach should be satisfied for any function $u(x, 0)$. Thus the problem is equivalent to finding an approximation to the Dirac distribution function δ as

$$\delta(x-t) \simeq \lim_{s \to 0} \left(\sum_{j=1}^{n} a_j(x, 0)\, P(x_j - t, s) + \sum_{k=n+1}^{n+m} b_k(x, 0) \frac{\partial P(x_k - t, s)}{\partial s} \right). \tag{9}$$

It is known that the Fourier transform with respect to the variable x of Poisson's kernel is $e^{-y\|w\|}$. By taking Fourier transform with respect to the variable t on both sides of Eq. (9) and letting s tend to zero, we obtain

$$e^{ixw} \simeq \sum_{j=1}^{n} a_j(x, 0)\, e^{ix_j w} - \sum_{k=n+1}^{n+m} |w|\, b_k(x, 0)\, e^{ix_k w}. \tag{10}$$

The problem is now confined to finding free functions $a_j(x, 0)$ and $b_k(x, 0)$ to make the approximation (10) precise. To achieve this we take a weighted linear approximation with a weight function $\hat{\phi}(w) > 0$, and for every fixed x, we determine $a_j(x, 0)$ and $b_k(x, 0)$ such that the value of the functional

$$I = \int \left| \sum_{j=1}^{n} a_j(x, 0)\, e^{ix_j w} - |w| \sum_{k=n+1}^{n+m} b_k(x, 0)\, e^{ix_k w} - e^{ixw} \right|^2 \hat{\phi}(w)\, dw \tag{11}$$

is minimized. Here, we assume that the weight function $\hat{\phi}(w)$ is a radial function (isotropy). The kernel function is then defined to be

$$\phi(x, y) = \int_{R^d} \int_{R^d} P(x-t, y)\, e^{-itw} \hat{\phi}(w)\, dw\, dt.$$

By using Lagrange's method, the minimizing problem (11) is equivalent to solving a linear system of equations

$$A \begin{pmatrix} a_j(x, 0) \\ b_k(x, 0) \end{pmatrix} = \begin{pmatrix} \phi(x - x_j, 0) \\ \dfrac{\partial \phi(x - x_k, 0)}{\partial y} \end{pmatrix}, \tag{12}$$

where A is a $(n+m) \times (n+m)$ matrix given as

$$A = \begin{pmatrix} \phi(x_k - x_j, 0) & \dfrac{\partial \phi(x_k - x_j, 0)}{\partial y} \\ \dfrac{\partial \phi(x_k - x_j, 0)}{\partial y} & \dfrac{\partial^2 \phi(x_k - x_j, 0)}{\partial y^2} \end{pmatrix}. \tag{13}$$

From Poisson's integral representation we can obtain $a_j(x, y)$ and $b_k(x, y)$ from $a_j(x, 0)$ and $b_k(x, 0)$. The approximated solution is finally given as

$$u^*(x, y) = (f^T, g^T)\, A^{-1} \begin{pmatrix} \phi(x-x_j, y) \\ \dfrac{\partial \phi(x-x_j, y)}{\partial y} \end{pmatrix}. \tag{14}$$

We have then shown that the problem is reduced to finding the multiple integrals of a pre-determined kernel function $\phi(x-x_j, y)$ and its partial derivative $\partial\phi(x-x_j, y)/\partial y$, which can be performed by using any approximation scheme for multiple integrals. Once these multiple integrals have been obtained, the multiple integral of the unknown solution $u(x, y)$ given in (2) can be achieved by using the approximation (14) which depends only on the given Cauchy data $f(x_j)$ and $g(x_k)$ and the pre- determined multiple integral values.

Summarizing the discussion above, we get another (dual) representation of the solution

$$u^*(x, y) = \sum_{j=1}^{n} \lambda_j \phi(x-x_j, y) + \sum_{k=n+1}^{n+m} \mu_k \frac{\partial \phi(x-x_k, y)}{\partial y},$$

where λ_j and μ_k are the solutions of the following linear system of equations

$$A \begin{pmatrix} \lambda_j \\ \mu_j \end{pmatrix} = \begin{pmatrix} f(x_k) \\ g(x_k) \end{pmatrix}.$$

In this dual representation it is only required to solve one linear system of equations (unlike (11), where the minimizing process must be taken for every fixed x). The existence and uniqueness of the solution depend on the non-singularity of the coefficient matrix A and can be proven by the following theorem.

THEOREM 1.1. *If the knots $\{x_j\}$ and $\{x_k\}$ are two sets of pairwisely distinct points, the function $\phi(x, y)$ is defined by the above Poisson's integral, and $\phi(x, 0)$ is a positive definite function respect to the variable x (equivalently $\hat{\phi}(w) > 0$ by Bohner's Theorem), then the matrix A is positive definite and non-singular.*

Proof. The Fourier transform with respect to the variable x of the Poisson's kernel is

$$\hat{P}(w, y) = e^{-y|w|}.$$

Using Poisson's integral representation of the harmonic functions ϕ and Parseval's Identity in the Fourier transform theory (see [2, 11] for reference), we obtain

$$\begin{aligned}\phi(x, y) &= \int_{R^d} P(x-t, y)\, \phi(t, 0)\, dt, \\ &= \int_{R^d} e^{-y|w|} \hat{\phi}(w)\, e^{-ixw}\, dw.\end{aligned}$$

By taking the derivatives of ϕ with respect to the variable y and letting y tend to zero, we have

$$\phi(x, 0) = \int_{R^d} e^{-ixw} \hat{\phi}(w)\, dw,$$

$$\frac{\partial \phi(x, 0)}{\partial y} = -\int_{R^d} e^{-ixw} \hat{\phi}(w)\, |w|\, dw,$$

and

$$\frac{\partial^2 \phi(x, 0)}{\partial y^2} = \int_{R^d} e^{-ixw} \hat{\phi}(w)\, |w|^2\, dw.$$

Since $\{e^{-ix_j w}, |w|\, e^{-ix_k w}\}$ are linearly independent for pairwisely distinct points $\{x_j\}_{j=1}^{n}$ and $\{x_k\}_{k=n+1}^{n+m}$, the following inequality holds strictly for any non-zero vectors λ and μ:

$$(\lambda^T, \mu^T)\, A \begin{pmatrix} \lambda \\ \mu \end{pmatrix} = \int_{R^d} \left| \sum_{j=1}^{n} \lambda_j e^{-ix_j u} - |w| \sum_{k=n+1}^{n+m} \mu_k e^{-ix_k w} \right|^2 \hat{\phi}(w)\, dw > 0.$$

It follows that the matrix A is positive definite and hence non-singular. ∎

3. ERROR ESTIMATION

Applying the Poisson's integral representation to both sides of equation (12), we obtain

$$A\begin{pmatrix} a_j(x, y) \\ b_k(x, y) \end{pmatrix} = \begin{pmatrix} \phi(x-x_j, y) \\ \dfrac{\partial \phi(x-x_k, y)}{\partial y} \end{pmatrix}. \tag{15}$$

Taking partial derivative with respect to the variable y to both sides of Eq. (15), we get

$$A\begin{pmatrix} \dfrac{\partial a_j(x, y)}{\partial y} \\ \dfrac{\partial b_k(x, y)}{\partial y} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \phi(x-x_j, y)}{\partial y} \\ \dfrac{\partial^2 \phi(x-x_k, y)}{\partial y^2} \end{pmatrix}. \tag{16}$$

Again, taking partial derivative with respect to the variable x to both sides of Eq. (15), we get

$$A\begin{pmatrix} \dfrac{\partial a_j(x, y)}{\partial x} \\ \dfrac{\partial b_k(x, y)}{\partial x} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \phi(x-x_j, y)}{\partial x} \\ \dfrac{\partial^2 \phi(x-x_k, y)}{\partial x\, \partial y} \end{pmatrix}. \tag{17}$$

Let $y = 0$ in both Eqs. (16) and (17). For every fixed x, the set of functions $(\partial a_j(x, 0)/\partial y, \partial b_k(x, 0)/\partial y)$ minimizes the functional

$$I_y = \int \left| \sum_{j=1}^{n} \frac{\partial a_j(x, 0)}{\partial y} e^{ix_j w} - \sum_{k=n+1}^{n+m} |w| \frac{\partial b_k(x, 0)}{\partial y} e^{ix_k w} + |w|\, e^{ixw} \right|^2 \hat{\phi}(w)\, dw,$$

and the set of functions $(\partial a_j(x, 0)/\partial x, \partial b_k(x, 0)/\partial x)$ minimizes the functional

$$I_x = \int \left| \sum_{j=1}^{n} \frac{\partial a_j(x, 0)}{\partial x} e^{ix_j w} - \sum_{k=n+1}^{n+m} |w| \frac{\partial b_k(x, 0)}{\partial x} e^{ix_k w} - iwe^{ixw} \right|^2 \hat{\phi}(w)\, dw,$$

respectively. Define the density of the sampling knots $\{x_j\}$ by

$$h = \max_{x \in [0,1]^d} \left\{ \min_{j=1}^{n} \{\|x - x_j\|\}, \min_{k=n+1}^{n+m} \{\|x - x_k\|\} \right\}.$$

The approximation to the solution is then the solutions of the linear systems of Eqs. (12), (16), and (17) which minimize the functionals I, I_x, and I_y, respectively. From the results given by Wu and Schaback [13, 14], the error bounds are $I = O(h^m)$, $I_x = O(h^{m-2})$ and $I_y = O(h^{m-2})$, respectively, if $\hat{\phi}(w) \sim (1+|w|)^{-m-d}$. The error estimation for the proposed method is then concluded as

THEOREM 2.1. *If the solution $u(x, y)$ satisfies $u(x, 0) \in C^l$, then we can choose a harmonic function $\phi(x, y)$ such that $\hat{\phi}(w) \sim (1+|w|)^{-m-d}$ and $\phi(x, 0)$ is a positive definite function, where $2l > m$. The errors on the boundary can be estimated as*

$$\|u^*(x, 0) - u(x, 0)\|^2_{H^1[0,1]} \leqslant ch^{m-2},$$

and

$$\left\| \frac{\partial u^*(x, 0)}{\partial y} - \frac{\partial u(x, 0)}{\partial y} \right\|^2_{L^2[0,1]} \leqslant ch^{m-2},$$

where the constant c depends only on the function $\phi(x, y)$ and the solution $u(x, y)$ but not on the density h of the knots. Furthermore, by using the results in [4], *we can obtain*

$$\int_{[0,1]} \int_{[-1,1]^d} (u^*(x, y) - u(x, y))^2 \, dx \, dy \leqslant \frac{c}{\log h^{m-2}}$$

for $d \leqslant 3$.

Remark 2.1. Our discussion above is for functions which are bounded (a condition of Bukhgeim's theorem) and harmonic on the upper half plane. The numerical results given in the next section, however, indicate that the method can be applied to unbounded functions.

4. NUMERICAL RESULTS

For numerical verification of the proposed method, we first construct a harmonic function by taking the real part of the complex function $e^{-\alpha z^2}$ so

that the function $\phi(x, y) = e^{-\alpha x^2 + \alpha y^2} \cos(2\alpha xy)$ is harmonic on the upper half plane and is the commonly used Gaussian function when $y = 0$ ($\phi(x, 0) = e^{-\alpha x^2}$) in the method of kriging. The approximation to the solution of the problem is then

$$u^*(x, y) = \sum_{j=1}^{n} \lambda_j \phi(x - x_j, y) + \sum_{j=n+1}^{n+m} \mu_j \frac{\partial \phi(x - x_j, y)}{\partial y},$$

where the collocation conditions

$$\sum_{k=1}^{n} \lambda_k \phi(x_j - x_k, 0) = f(x_j), \qquad j = 1, \ldots, n,$$

and

$$\sum_{k=n+1}^{n+m} \mu_k \phi''(x_j - x_k, 0) = g(x_j), \qquad j = n+1, \ldots, n+m,$$

must be satisfied because all the first order partial derivatives of the real part of the Gaussian kernel function ϕ with respect to the variable y on the boundary is zero. This is an advantage of using the Gaussian kernel function in dividing the linear system of equations of order $n+m$ into two smaller linear systems of equations of orders n and m, respectively, which is not valid for arbitrary kernel function. The numerical results show that this linear scheme provides a good approximation to the solution of the problem.

Other than the above Gaussian kernel, we have also tested the applicability and accuracy of the method by using the following kernel functions: ($c > 0$)

(1) Gaussian: $\phi_1(x, y) = e^{-(x^2 - y^2)/c} \cos(2xy/c)$, $\phi_1(x, 0) = e^{-x^2/c}$,

(2) Multiquadric: $\phi_2(x, y) = Re(\sqrt{c^2 + z^2})$, $\phi_2(x, 0) = \sqrt{c^2 + x^2}$,

(3) Poisson kernel: $\phi_3(x, y) = y/(x^2 + (y + c)^2)$, $\phi_3(x, 0) \sim \delta(x)$.

In our numerical verifications, we choose the solution $u(x, y)$ to be the commonly used harmonic function $u(x, y) = x^2 - y^2 +$ any degree one polynomial and functions of the form $\phi_1(x, y)$, $\phi_2(x, y)$, and $\phi_3(x, y)$ with different values of c in the range $[0.01, 100]$. The Table I lists the numerical

TABLE I

Average Errors by Using Different Kernel Functions

Type	Kernel function	Absolute maximum error
Gaussian	Real part of $e^{-0.1z^2}$	$6.3761*10^{-5}$
Gaussian	Real part of $e^{-0.01z^2}$	$4.1475*10^{-6}$
Multiquadric	Real part of $\sqrt{9^2+z^2}$	$1.7571*10^{-5}$
Multiquadric	Real part of $\sqrt{6^2+z^2}$	$2.7410*10^{-5}$
Multiquadric	Real part of $\sqrt{3^2+z^2}$	$4.4904*10^{-4}$
Poisson	$\frac{y}{x^2+(y+2)^2}$	$3.2572*10^{-4}$
Poisson	$\frac{y}{x^2+(y+4)^2}$	$1.7036*10^{-4}$

results by using some of the above kernel functions to be the predetermined function $\phi_j(x, y)$ in the approximation formula (14) for $u^*(x, y)$. In Table I, the absolute maximum error ($AMErr$) is defined by

$$AMErr = \max_{u} \max_{x, y} |u(x, y) - u^*(x, y)|. \tag{18}$$

All the numerical computations are performed in a PC with the standard matrix solver MATLAB.

In all of the computations, the problem is defined in the region $[-1, 1] \times [0, 1]$ and the data points are chosen uniformly from $[-1/2, 1/2] \times [0, 0]$ with density $h = 10^{-1}$. It can be observed from Table I that all the absolute maximum errors between the multiple integrals of the solution $u(x, y)$ and the approximant $u^*(x, y)$ lie between 10^{-6} and 10^{-4}. It is clear that the multiple integral error will not exceed twice of the absolute maximum error given in Table I.

Remark 3.1. By adjusting the parameters α and c contained in the kernel functions, we can obtain even better numerical approximations. All the numerical results indicate that the errors of approximation are monotonically decreasing as the parameter c increases until the coefficient matrices are not computable due to large condition numbers. This restriction is also observed when using the radial basis functions for scattered data interpolation and solutions of partial differential equations.

Remark 3.2. The results given in this paper are for those harmonic functions which can be represented by Poisson's integral. By using the technique of harmonic map, the approach can be extended to functions which are harmonic on a bounded domain, providing that the domain is an image of the upper half plane by the harmonic map.

ACKNOWLEDGMENTS

The first author thanks the Organizers of the International Conference on Complexity, 1999, who supported him in presenting his talk at the Conference. The authors also thank the editors and referees for their valuable suggestions.

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